

A UNIVERSALITY THEOREM FOR NONNEGATIVE MATRIX FACTORIZATIONS

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ABSTRACT. Let A be a matrix with nonnegative entries in an ordered field \mathcal{F} . The nonnegative factorization of size k is a representation of A as a sum of k nonnegative rank-one matrices. The space of all such factorizations is a bounded semialgebraic set, and we prove that the spaces arising in this way are universal. More precisely, we show that every bounded semialgebraic set U is rationally equivalent to the set of nonnegative size- k factorizations of a matrix A up to a permutation of matrices in the factorization. We prove that, if $U \subset \mathbb{R}$ is given as the zero locus of some polynomial with coefficients in \mathbb{Q} , then such a pair (A, k) can be computed in polynomial time. This result allows us to determine the computational complexity status of the nonnegative rank and solve several other open problems in the theory of nonnegative matrices.

1. THE FORMULATION

The goal of this paper is to prove the universality theorem for spaces of nonnegative matrix factorizations. The goal of this section is to introduce the concepts that appear in this theorem and formulate it. We fix an ordered field \mathcal{F} and a real closed field \mathcal{R} containing \mathcal{F} , and we use these symbols throughout the paper as a designation of these fields. For instance, if we assume that $\mathcal{F} = \mathbb{Q}$, then we can assume $\mathcal{R} = \mathbb{R}$. We denote by \mathcal{F}_+ the set of all nonnegative elements of \mathcal{F} , and we call a matrix A over \mathcal{F} nonnegative if its entries belong to \mathcal{F}_+ . A nonnegative k -factorization of such a matrix is a family (A_1, \dots, A_k) of rank-one matrices with entries in \mathcal{R}_+ such that $A_1 + \dots + A_k = A$. Any permutation of this family still leads to a valid factorization, but we do not want to think of these factorizations as different ones.

We define $\text{fact}_+(A, k)$ as the set of all nonnegative k -factorizations of A satisfying an additional assumption that $A_1 \succ \dots \succ A_k$, where \succ denotes the lexicographic ordering on the set of matrices. Clearly, the set $\text{fact}_+(A, k)$ is a bounded semialgebraic subset of \mathcal{R}^{mnk} , where m and n are the dimensions of the matrix A . That is, this set can be defined by a quantifier-free formula over \mathcal{F} , and the entries of matrices in the factorizations are bounded by some constant (namely, by the maximal entry of A). The *nonnegative rank* of A is the smallest k such that $\text{fact}_+(A, k)$ is non-empty; we denote this quantity by $\text{rk}_+(A)$.

Consider sets $U \subset \mathcal{R}^n$ and $V \subset \mathcal{R}^m$ such that $\pi(V) = U$, where $\pi : \mathcal{R}^m \rightarrow \mathcal{R}^n$ denotes the natural projection onto the first n ($\leq m$) coordinates. Assume that there are functions $\varphi_1, \dots, \varphi_m$ rational over \mathcal{F} such that, for all $u = (u_1, \dots, u_n) \in U$,

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the preimage $\pi^{-1}(u)$ is unique and equal to

$$(u_1, \dots, u_n, \varphi_{n+1}(u), \dots, \varphi_m(u)).$$

In this case, we say that π is a *rational projection* between U and V . A *permutation mapping* from \mathcal{R}^n to \mathcal{R}^n is a mapping that is defined, for any permutation σ on n elements, as $(a_1, \dots, a_n) \rightarrow (a_{\sigma(1)}, \dots, a_{\sigma(n)})$. We say that arbitrary sets $U_1 \subset \mathcal{R}^n$ and $U_2 \subset \mathcal{R}^m$ are *almost equal* if (U_1, U_2) belongs to the equivalence relation generated by rational projections and permutation mappings. In particular, we can see that any two almost equal sets are rationally equivalent as well.

The goal of this paper is to prove the result which characterizes spaces of non-negative matrix factorizations as semialgebraic sets. Our theorem is related to the famous universality theorem of Mnëv [11] on oriented matroids. Let us also mention the universality theorems for polytopes [12] and Nash equilibria [7].

The Universality Theorem for Nonnegative Factorizations.

Let F be the zero locus of a polynomial $f \in \mathcal{F}[x_1, \dots, x_n]$.

There are a matrix M over \mathcal{F}_+ and an integer k such that $\text{fact}_+(M, k)$ is almost equal to $F \cap [0, 1]^n$. If $\mathcal{F} = \mathbb{Q}$, then one can find M and k in polynomial time¹.

Our paper is structured as follows. In Section 2, we introduce a gadget that allows us to replace some entries in the matrices with unknowns, which leads to a problem richer than the conventional NMF. In Section 3, we make use of this gadget and reduce a more general problem to NMF. We complete the proof of the Universality theorem in Section 4, and we discuss the applications of this theorem in Section 5.

2. THE “VARIABLE GADGET”

In this section we explain the connection between the classical NMF problem and its generalization in which the matrices are allowed to contain unknown entries. In other words, we consider so called *incomplete matrices* which may contain not only elements of \mathcal{F}_+ but also variables whose ranges are segments in \mathcal{F}_+ . Let \mathcal{A} be such a matrix; a completion of \mathcal{A} is a matrix that can be obtained from \mathcal{A} by assigning some value to every variable within its range. We define $\text{fact}_+(\mathcal{A}, k)$ as the union of all sets $\text{fact}_+(A, k)$ over all completions A of \mathcal{A} . The smallest k for which $\text{fact}_+(\mathcal{A}, k)$ is non-empty is called the *nonnegative rank* of an incomplete matrix \mathcal{A} . Let us illustrate the given definitions with an example.

Example 1. Consider the incomplete matrix

$$\mathcal{A} = \begin{pmatrix} y & 0 & 0 \\ 0 & x & 2 \\ 0 & 1 & x \end{pmatrix},$$

with $x \in [0, 1]$ and $y \in [1, 2]$. Every completion of \mathcal{A} is a block-diagonal matrix with non-singular blocks, so we get $\text{rk}_+(\mathcal{A}) = 3$. Despite this fact, we note that the values $x = \sqrt{2}$ and $y = 0$ would produce a matrix with nonnegative rank one, but we are not allowed to assign values which do not belong to corresponding ranges.

Now we turn to the description of our gadget. We begin with a standard example.

¹When we discuss the computational complexity, we assume that the polynomial f is written in the *standard form* as a sum of monomials with coefficients and exponents written in the unary.

Proposition 2. [13] *Let*

$$V = \begin{pmatrix} 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & 1 \end{pmatrix}.$$

One has $\text{rk}_+(V) = 4$.

Further, we generalize the example as in [15].

Proposition 3. *Let u_1, \dots, u_n be nonnegative reals ($n \geq 1$). Every nonnegative 4-factorization of the matrix*

$$\mathcal{V}(u_1, \dots, u_n) = \begin{pmatrix} 1 & 1 & 0 & 0 & 0 & \dots & 0 \\ 0 & 1 & 1 & 0 & 0 & \dots & 0 \\ 0 & 0 & 1 & 1 & 0 & \dots & 0 \\ 1 & 0 & 0 & 1 & 1 & \dots & 1 \\ 1 & 1 & 1 & 1 & u_1 & \dots & u_n \end{pmatrix}$$

has the form

$$\begin{pmatrix} V_1 \\ O \\ O \\ O \\ (1-u_1)V_1 \end{pmatrix} + \begin{pmatrix} O \\ V_2 \\ O \\ O \\ u_1V_2 \end{pmatrix} + \begin{pmatrix} O \\ O \\ V_3 \\ O \\ (1-u_1)V_3 \end{pmatrix} + \begin{pmatrix} O \\ O \\ O \\ V_4 \\ u_1V_4 \end{pmatrix},$$

where V_i denotes the i th row of the matrix $\mathcal{V}(u_1, \dots, u_n)$, and O is the zero row. In particular, we have $\text{rk}_+(\mathcal{V}) = 4$ if $u_1 = \dots = u_n \in [0, 1]$ and $\text{rk}_+(\mathcal{V}) = 5$ otherwise.

Proof. Straightforward. \square

Now we present the gadget pointing out the connection between the classical NMF problem and the corresponding problem for incomplete matrices. Let

$$A = \left(\begin{array}{c|ccc} \overline{A} & & & B \\ \hline \textcolor{blue}{c} & \textcolor{blue}{N} & \dots & \textcolor{blue}{N} \end{array} \right)$$

be a nonnegative matrix. We will say that the matrix

$$G = \left(\begin{array}{c|ccc|cccc} \overline{A} & & & B & 0 & 0 & 0 & 0 \\ \hline \textcolor{blue}{c} & \textcolor{blue}{N} & \dots & \textcolor{blue}{N} & \textcolor{green}{M} & \textcolor{green}{M} & \textcolor{green}{M} & \textcolor{green}{M} \\ \hline 0 & \dots & 0 & \textcolor{green}{M} & \dots & \textcolor{green}{M} & \textcolor{red}{M} & \textcolor{red}{M} & 0 & 0 \\ 0 & \dots & 0 & 0 & \dots & 0 & 0 & \textcolor{red}{M} & \textcolor{red}{M} & 0 \\ 0 & \dots & 0 & 0 & \dots & 0 & 0 & 0 & \textcolor{red}{M} & \textcolor{red}{M} \\ 0 & \dots & 0 & 0 & \dots & 0 & \textcolor{red}{M} & 0 & 0 & \textcolor{red}{M} \end{array} \right)$$

is obtained from A by applying the *variable gadget with parameter M* to the blue entries. Let \mathcal{A} be the matrix obtained from A by replacing the blue entries with a variable x ranging in $[\max\{0, N - M\}, N]$. We have the following proposition.

Proposition 4. *If $M, N \in \mathcal{F}_+$ and*

$$\text{rk}_+(\overline{A} \mid \textcolor{blue}{B}) \geq r \quad \text{and} \quad \text{rk}_+\left(\frac{\overline{A}}{\textcolor{brown}{c}}\right) \geq r,$$

then $\text{fact}_+(G, r+4)$ and $\text{fact}_+(\mathcal{A}, r)$ are almost equal.

Proof. By Proposition 2, any nonnegative factorization of G contains four matrices with non-zero red entries. These matrices do not contribute to anything in A except possibly a blue entry, so if the factorization has $r+4$ matrices, every other matrix has a non-zero black entry (or both a non-zero light blue entry and a non-zero yellow entry, which still implies the existence of a non-zero black entry). Therefore, there are exactly four matrices in this factorization that contribute to red and green entries, and these four matrices can be determined by Proposition 3. \square

3. A STRONGER “VARIABLE GADGET”

Let B be an incomplete matrix whose entries are elements of \mathcal{F}_+ and variables x, x_1, \dots, x_n . We denote the set of entries equal to x by $\mathcal{T} = \{(i_1, j_1), \dots, (i_\tau, j_\tau)\}$, and we assume that the sequences i_1, \dots, i_τ and j_1, \dots, j_τ do not contain repeating indexes. Assume $M, N, P, Q \in \mathcal{F}$ are such that $N \geq Q \geq P > 0$ and $M \geq 1/P$. We construct the matrix

$$\left(\begin{array}{cccc|ccc|ccc} \textcolor{red}{N} & \textcolor{red}{N} & 0 & 0 & & & & & & & \\ 0 & \textcolor{red}{N} & \textcolor{red}{N} & 0 & & & & & & & \\ 0 & 0 & \textcolor{red}{N} & \textcolor{red}{N} & & & & & & & \\ \hline \textcolor{red}{N} & 0 & 0 & \textcolor{red}{N} & \textcolor{red}{N} & \dots & \textcolor{red}{N} & 0 & \dots & 0 & 0 & \dots & 0 \\ \textcolor{red}{N} & \textcolor{red}{N} & \textcolor{red}{N} & \textcolor{red}{N} & \textcolor{green}{N} & \dots & \textcolor{green}{N} & 1 & \dots & 1 & 0 & \dots & 0 \\ \hline & & & & \textcolor{blue}{QI}_\tau & & & I_\tau & & & O & & \\ \hline & & & & I_\tau & & & \textcolor{yellow}{B}_\mathcal{T} & & & B_2 & & \\ \hline & & & & O & & & B_3 & & & B_4 & & \end{array} \right)$$

and denote it by $\Gamma_1(B, x, M, N, P, Q)$. Here, the rows and columns of $\textcolor{yellow}{B}_\mathcal{T}$ have labels i_1, \dots, i_τ and j_1, \dots, j_τ , respectively, and the matrix $\begin{pmatrix} \textcolor{yellow}{B}_\mathcal{T} & B_2 \\ B_3 & B_4 \end{pmatrix}$ is obtained from B by replacing every entry equal to x by M . (Therefore, the diagonal entries of $\textcolor{yellow}{B}_\mathcal{T}$ become equal to M , and the matrix Γ_1 does not anymore depend on x .) We denote by $\Gamma(B, x, M, N, P, Q)$ the matrix obtained from Γ_1 by applying the variable gadgets with parameter $Q - P$ to every diagonal entry of the blue block $\textcolor{blue}{QI}_\tau$.

Proposition 5. *Let $\text{rk}_+(B_4) \geq \rho$ and $\rho' = \rho + 5\tau + 4$. Then $\text{fact}_+(\Gamma, \rho')$ and $\text{fact}_+(B, \rho)$ are almost equal, provided that $x \in [M - 1/P, M - 1/Q]$.*

Proof. Let Γ_2 be the matrix obtained from Γ_1 as follows. We remove the first four rows and the first four columns, we replace the green entries by the variable $c \in [0, N]$, we replace the diagonal entries of $\textcolor{blue}{QI}_\tau$ by different variables $v_i \in [P, Q]$. It can be seen from Proposition 4 that $\text{fact}_+(\Gamma, \rho')$ is almost equal to $\text{fact}_+(\Gamma_2, \rho + \tau)$.

Now let $(G_1, \dots, G_{\rho+\tau})$ be a nonnegative factorization of Γ_2 . We easily get $v_i = c$, and if G_j is a matrix with a non-zero blue entry, then it has to be equal to c , and we have $1/c$ at the corresponding entry of G_j located on the diagonal of the yellow block. So we can see that $\text{fact}_+(\Gamma_2, \rho + \tau)$ is almost equal to $\text{fact}_+(B, \rho)$, since $1/c = 1/v_i$ ranges in $[1/P, 1/Q]$. \square

The following theorem arises from a natural generalization of Proposition 5.

Theorem 6. *Let \mathcal{H} be an incomplete matrix whose entries are elements of \mathcal{F}_+ and variables x_1, \dots, x_n . Assume that x_i ranges in $[a_i, b_i] \subset \mathcal{F}_+$ and occurs at most once in every row and column. Let H_0 be the matrix obtained from \mathcal{H} by removing all the rows and columns in which the variables occur, and suppose $\text{rk}_+(H_0) = \rho_0$.*

Given these data, we can construct a complete matrix $\mathcal{M} = \mathcal{M}(\mathcal{H})$ and an integer ρ for which the sets $\text{fact}_+(\mathcal{M}, \rho)$ and $\text{fact}_+(\mathcal{H}, \rho_0)$ are almost equal. If $\mathcal{F} = \mathbb{Q}$, then we can find such \mathcal{M} and ρ in polynomial time.

Proof. Repeatedly apply Proposition 5 to eliminate variables x_1, \dots, x_n . \square

4. REPRESENTING A POLYNOMIAL EQUATION

In this section we complete the proof of the Universality theorem with the use of Theorem 6. The following lemmas explain how to express the polynomial equation $f = 0$ in terms of factorization spaces of partial matrices. Let us represent the equation involving a linear combination.

Lemma 7. *Let y_1, \dots, y_l be variables ranging in $[0, 1]$, let $s_1, \dots, s_l, N \in \mathcal{F}_+$ satisfy $N \geq s_1 + \dots + s_l$, and let L be a variable ranging in $[0, N]$. Let $S = S(s_1 y_1 + \dots + s_l y_l = L)$ be the matrix obtained from*

$$\left(\begin{array}{c|ccc} y_1 & & & \\ \vdots & & & \\ y_l & & & \\ \hline L & s_1 & \dots & s_l \\ \hline 1 & & & \\ \vdots & & & \\ 1 & & & \end{array} \begin{array}{c} I_l \\ \\ \\ \\ I_l \end{array} \right)$$

by applying the variable gadgets with parameter 1 to the blue entries. If we remove all the rows and columns of S which contain variables, we get a matrix with non-negative rank $5l$. For any fixed assignment of values to variables y_1, \dots, y_l , there is a unique nonnegative $5l$ -factorization of S corresponding to the value of L equal to $s_1 y_1 + \dots + s_l y_l$. Some entries of matrices in this factorization are equal to y_1, \dots, y_l , and the rest are rational functions of these variables fixed in advance.

Proof. Use Proposition 4 and replace the blue entries with variables. The rest is straightforward. \square

The following statement is similar to Lemma 7, and it allows us to multiply.

Lemma 8. *Let v, u_1, u_2 be variables ranging in $[0, 1]$. Let $P = P(u_1 u_2 = v)$ be the matrix obtained from*

$$\left(\begin{array}{ccc} \gamma & \alpha & 1 \\ \beta & 1 & 1 \\ 1 & 1 & 1 \end{array} \right)$$

by applying the variable gadgets with parameter 1 to the blue entries. If we remove all the rows and columns of S which contain variables, we get a matrix with nonnegative rank 9. For any fixed assignment of values to variables u_1, u_2 , there is a unique nonnegative 9-factorization of S corresponding to the value of v equal to $u_1 u_2$. Some entries of matrices in this factorization are equal to u_1, u_2 , and the rest are rational functions of these variables fixed in advance.

Proof. Use Proposition 4 and replace the blue entries with variables. The rest is straightforward. \square

Now we are ready to prove the Universality theorem. For any polynomial $f \in \mathcal{F}[x_1, \dots, x_n]$, we can write the equation $f = 0$ as $s_1 \mu_1 + \dots + s_l \mu_l = s_{l+1} \mu_{l+1} + \dots + s_r \mu_r$, where $s_i \in \mathcal{F}_+$ and μ_i are products of the form $\alpha_{i1} \dots \alpha_{im_i}$ with $\alpha_{ij} \in \{x_1, \dots, x_n\}$. We introduce new variables L and (v_{ij}) .

Now we are going to construct an incomplete matrix \mathcal{H} depending on the x_i 's, v_{ij} 's and L . As in the Lemmas 7 and 8, we assume that x_i 's and v_{ij} 's are ranging in $[0, 1]$, and also L is ranging in $[0, s_1 + \dots + s_r]$. We define \mathcal{H} as the block-diagonal matrix containing the following matrices as diagonal blocks: $S(L = s_1 v_{1m_1} + \dots + s_l v_{lm_l})$, $S(L = s_{l+1} v_{l+1, m_{l+1}} + \dots + s_r v_{rm_r})$, and all the matrices $P(v_{i2} = \alpha_{i1} \alpha_{i2})$ and $P(v_{ij} = v_{i, j-1} \alpha_{ij})$ for all i and all $j \in \{3, \dots, m_i\}$. (Here, we mean that v_{im_i} denotes the corresponding variable α_{i1} in the case $m_i = 1$.)

If we remove from \mathcal{H} all the rows and columns in which the variables occur, we get the matrix of nonnegative rank $\rho = 5r + 9(m_1 + \dots + m_r - r)$. By Lemmas 7 and 8, the set $\text{fact}_+(\mathcal{H}, \rho)$ is almost equal to the intersection of the cube $[0, 1]^n$ and the zero locus of f . It remains to apply Theorem 6 to complete the proof of the Universality theorem.

5. CONSEQUENCES OF THE UNIVERSALITY THEOREM

Let us consider a family of more specific rank functions; let A be a matrix with entries in \mathcal{F}_+ . Define $\text{rk}_+(A, \mathcal{F})$ as the smallest k such that $\text{fact}_+(A, k)$ contains a point with coordinates in \mathcal{F} ; this quantity is called the nonnegative rank of A with respect to \mathcal{F} . Cohen and Rothblum asked in [5], how sensitive is the nonnegative rank to the field with respect to which it is computed? We get the following answer to this question, generalizing the partial solutions in [4, 14, 15].

Corollary 9. *If $F \subsetneq K$ is an algebraic extension of ordered fields, then there is a matrix A over F such that $\text{Rank}_+(A, F) \neq \text{Rank}_+(A, K)$.*

Proof. Let $g = t^n + a_{t-1}t^{n-1} + \dots + a_0$ be the minimal polynomial of an element α in $K \setminus F$. We have $|\alpha| < q = n(|a_{t-1}| + \dots + |a_0| + 1)$, so we can apply UC with $f = g(2qt - q)$. \square

What is the complexity of computing the nonnegative rank with respect to different fields? Assume that $\mathcal{F} = \mathbb{Q}$ and consider the following decision problem: does a given bounded semialgebraic set contain a rational point? The Universality theorem (together with Theorem 11 below) shows that this problem is polynomial-time equivalent to computing the rational nonnegative rank. A notorious conjecture [9] states that the question of solubility of rational Diophantine equations is undecidable, so the current state of knowledge does not allow to compute $\text{Rank}_+(M, \mathbb{Q})$ algorithmically. We note that the question of decidability of rational nonnegative rank has been posed in [3].

Also, the Universality theorem allows us to determine the computational complexity status of the real nonnegative rank. Namely, the nonnegative rank is polynomial-time equivalent to the problem known as the *Existential theory of the reals* (ETR): Given a quantifier-free formula Φ over $(\mathbb{R}, +, -, *, 0, 1, =, >)$, is Φ satisfiable? This gives a complete resolution of the complexity status of the non-negative matrix factorization problem (NMF), which has been open despite the extensive discussion in the previous twenty years [1, 5, 17]. We note that NMF has been known to be NP-hard, see the original proof by Vavasis in [17] and a short proof in [16]. Several widely known references mention the result by Vavasis as an *NP-completeness* proof [1, 2, 6]; the following result shows that, however, NMF is unlikely to be NP-complete.

Corollary 10. *Real nonnegative rank is polynomial-time equivalent to ETR.*

In order to prove Corollary 10, we need the following results. One of them is a geometric result by Grigoriev and Vorobjov, and the other is an algorithmic proposition whose proof is essentially contained in the discussion of Proposition 3.2 in the paper [10] by Matousek.

Theorem 11. [8, Lemma 9] *Let L be the length of the formula expressing a polynomial $f \in \mathbb{Z}[x_1, \dots, x_n]$. Then every connected component V of the set $\{f = 0\}$ has a non-empty intersection with the ball of the radius $2^{2^{CL}}$ centered at the origin, where C is an absolute constant. If V is bounded, then V is contained in this ball.*

Theorem 12. *There exists a linear-time algorithm sending a quantifier-free formula $\Phi(x_1, \dots, x_n)$ to an equivalent formula $\exists x_{n+1} \dots \exists x_m \pi(x_1, \dots, x_m) = 0$ in which π is a polynomial written in the standard form.*

Now we are ready to deduce Corollary 10 from the Universality theorem. By Theorem 12, ETR is polynomially equivalent to its restricted version in which Φ is a single polynomial equation $f(x_1, \dots, x_n) = 0$. Denoting the length of f by L , we set $\sigma = \lceil CL \rceil + 1$ and $s = 2^{-2^\sigma}$. We define

$$h(x_0, \dots, x_n) = x_0^d \cdot f\left(\frac{2x_1 - 1}{x_0}, \dots, \frac{2x_n - 1}{x_0}\right),$$

where x_0 is a new variable and d is the degree of f . Introducing new variables s_0, \dots, s_σ , we set

$$g = (2s_0 - 1)^2 + \sum_{j=0}^{\sigma-1} (s_{j+1} - s_j^2)^2 + (x_0 - s_\sigma)^2 + h^2$$

and denote by G the zero locus of g . We apply the Universality theorem to the polynomial g , and construct a matrix M and an integer k such that the condition $\text{rk}_+(M, \mathbb{R}) \leq k$ is equivalent to the solubility of the equation $g = 0$. The first three summands in the equation $g = 0$ tell us that $s_k = 2^{-2^k}$ and $x_0 = s_\sigma = s$. Therefore, G has a non-empty intersection with the cube $[0, 1]^n$ if and only if h has a solution in this cube with $x_0 = s$. By the definition of h , this happens if and only if $f = 0$ has a solution in $[-1/s, 1/s]^n$, and this is equivalent to the solubility of $f = 0$ by Theorem 11. Corollary 10 follows.

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